

# Nematicity at the Hund's metal crossover in iron superconductors

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The theoretical understanding of the nematic state of iron-based superconductors and especially of FeSe is still a puzzling problem. Although a number of experiments calls for a prominent role of local correlations and place iron superconductors at the entrance of a Hund metal state, the effect of the electronic correlations on the nematic state has been theoretically poorly investigated. In this work we study the nematic phase of iron superconductors accounting for local correlations, including the effect of the Hund's coupling. We show that Hund's physics strongly affects the nematic properties of the system. It severely constraints the precise nature of the feasible orbital-ordered state and induces a differentiation in the effective masses of the  $zx/yz$  orbitals in the nematic phase. The latter effect leads to distinctive signatures in different experimental probes, so far overlooked in the interpretation of experiments. As notable examples the splittings between  $zx$  and  $yz$  bands at  $\Gamma$  and M points are modified, with important consequences for ARPES measurements.

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## INTRODUCTION

The nematic state is one of the most debated issues in iron-based superconductors (IBS) [1–4]. Perturbative approaches which attribute the ordered phases to Fermi-surface instabilities have succeeded in explaining many properties of IBS, including the occurrence of a nematic phase. Within this framework, the Ising spin-nematic model [2, 5–8], interpreted the nematic state as a precursor of the  $(\pi, 0)$  stripe order.

On the other hand, many theoretical studies [9–22] have highlighted the relevance of electron correlations driven by local interactions, and in particular by the Hund's coupling, to explain the bad metallic behavior of the normal state of IBS. A number of experimental investigations support indeed this scenario [20, 23–26].

Several theoretical investigations agree on a central role of the Hund's coupling and link the phenomenology of IBS to a crossover between a normal metal and the so-called Hund's metal which occurs when the interactions are increased. In particular, the IBS lie close to this crossover, which is characterized by a suppression of the overall coherence of conduction electrons and it is accompanied by a pronounced differentiation of the correlation strengths between different orbitals [20, 21]. As a matter of fact the system appears in this region particularly sensitive to any kind of perturbation. Therefore accounting for local correlations is crucial for any realistic theoretical study of the nematic phase of IBS.

The nematic state of FeSe deserves a particular interest. Even if sizable spin fluctuations have been detected [31–33], the lack of magnetic order in this material casts doubts on a magnetic origin of nematicity challenging the Ising spin-nematic picture. This has reinvigorated approaches based on orbital ordering. Orbital order models have mostly focused on states with occupation imbalance

between  $zx$  and  $yz$  orbitals [34–37]. However calculations on realistic IBS tight-binding models using FLEX [38] and Hartree-Fock methods [39, 40] do not find a similar instability. In fact Hund's coupling favors an even population of the orbitals in order to maximize the spin.

More recently, it has been proposed that FeSe can host orbital ordering with  $n_{zx} \neq n_{yz}$  mediated by spin fluctuations because of the relatively small ratio between Hund's coupling  $J_H$  and intraorbital interactions  $U$  [41]. This argument however neglects that FeSe is one of the most correlated IBS [13, 19, 22] as testified by the recent observation of the Hubbard bands [42, 43], the large mass enhancements [28–30] and the orbital-dependent coherence-incoherence crossover [23], features typical of Hund's metals. The value of  $U$ , larger in FeSe than in other IBS [44] makes Hund's physics relevant in FeSe despite a smaller  $J_H/U$  ratio and requires including the correlations beyond the approximation used in [41].

Besides the onsite ferro-orbital ordering (OFO) discussed above, other orbital orders have been proposed to explain the nematic state of FeSe. In particular: (i) An orbital polarization with sign reversal between electron (e) and hole (h) pockets ("sign-changing bond order", SCO) emerges from parquet renormalization group (RG) calculations when the Fermi energy is small, as in FeSe [45]; (ii) A nematic d-wave bond order (DBO) [46] stabilized by a large intersite repulsion [47], was proposed to explain early ARPES experiments in FeSe [29, 30, 48–50], which at present are controversial [51–53].

The predictions for the stability and the spectroscopic signatures of the orbital-ordered states discussed so far are based on techniques unable to address the effect of local correlations and could change once Hund's physics is taken into account. In this work we study the impact of short-range correlations on the anisotropic properties of IBS in the nematic state including the possibility that

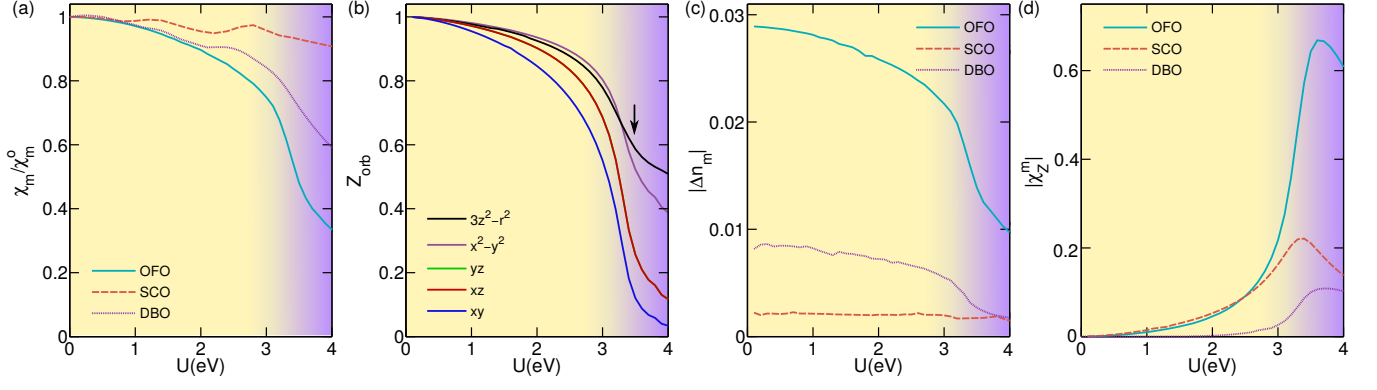


FIG. 1: (Color online)(a) Orbital nematic susceptibilities  $\chi_m(U)$  normalized to their respective  $U = 0$  value, for  $J_H/U = 0.20$  and electronic filling  $n = 6$  [27]. The OFO is strongly suppressed by interactions while the SCO is only weakly affected. (b) Orbital-dependent quasiparticle weight  $Z_\gamma$  as a function of  $U$  in the absence of a nematic perturbation. The sharp drop around  $U \sim 3.2$  eV signals the entrance into the strongly correlated Hund's metal region where the atoms become spin polarized. The shading colors in the panels differentiate the weakly correlated and the Hund's metal regime. The arrow signals the interaction value  $U = 3.5$  eV at which the orbital-dependent mass enhancements equal those observed in ARPES and Quantum Oscillations experiments in FeSe [28–30]. (c) Occupation imbalance between  $xz$  and  $yz$  orbitals for the three orders taking  $2h_m = 75\text{meV}$ . The larger is the imbalance produced by an order, the stronger is the  $\chi_m(U)$  suppression of this order by interactions. (d) Absolute value of the Z-response functions  $\chi_Z^m(U)$ .

local correlations induce a phase transition to an orbital-ordered state. We use slave-spin calculations to study whether Hund's physics coexist or compete with three different orbital orders: onsite ferro-orbital order OFO, SCO which changes sign between the e/h-pockets and d-wave bond nematic order DBO. We find that: (i) Local correlations alone are not able to stabilize a nematic orbital phase but constraints the nature of the possible orbital orders. In particular Hund's coupling strongly suppresses those orders which produce larger uneven occupation of  $xz$  and  $yz$  orbitals, as the OFO, but it has a minor effect on the orders for which the occupation imbalance is small, as the SCO; (ii) The orbital decoupling induced by interactions at the Hund's metal crossover favors a differentiation of the  $xz/yz$  orbitals masses in the nematic phase; (iii) Interactions modify the orbital splittings between  $yz$  and  $xz$  at the  $\Gamma$  and  $M$  symmetry points with strong implications in the interpretation of ARPES experiments.

### THE MODEL

We consider a five-orbital Hubbard-Kanamori Hamiltonian, widely used to study IBS

$$\begin{aligned}
 H = & \sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c_{i,\gamma,\sigma}^\dagger c_{j,\beta,\sigma} + h.c. + U \sum_{j,\gamma} n_{j,\gamma,\uparrow} n_{j,\gamma,\downarrow} \\
 & + (U' - \frac{J_H}{2}) \sum_{j,\gamma > \beta, \sigma, \tilde{\sigma}} n_{j,\gamma,\sigma} n_{j,\beta,\tilde{\sigma}} - 2J_H \sum_{j,\gamma > \beta} \vec{S}_{j,\gamma} \vec{S}_{j,\beta} \\
 & + J' \sum_{j,\gamma \neq \beta} c_{j,\gamma,\uparrow}^\dagger c_{j,\gamma,\downarrow}^\dagger c_{j,\beta,\downarrow} c_{j,\beta,\uparrow} + \sum_{j,\gamma,\sigma} \epsilon_\gamma n_{j,\gamma,\sigma}. \quad (1)
 \end{aligned}$$

$i, j$  label the Fe sites in the 1-Fe unit cell,  $\sigma$  the spin and  $\gamma, \beta$  the five Fe d-orbitals  $yz, zx, xy, 3z^2 - r^2$  and  $x^2 - y^2$ , with  $x$  and  $y$  axis along the Fe-Fe bonds. For the tight-binding Hamiltonian we refer to the parameters used in [20] for FeSe.  $U$  and  $U'$  are the intra- and inter-orbital interactions,  $J_H$  is the Hund's coupling and  $J'$  the pair-hopping and we assume  $U' = U - 2J_H$ . Except otherwise indicated we use  $J_H = 0.2U$  and electronic filling  $n = 6$  as in undoped IBS. We consider only the density-density part of the interaction, that we treat with the single-site slave spin mean-field [21, 54–56]. This method accounts for the effect of local correlations, and gives the correlated value of the orbital dependent fillings  $n_\gamma$  and mass enhancements which produces the band narrowing observed experimentally. At the single-site level used here, the mass enhancements equal the inverse of the quasiparticle spectral weights  $Z_\gamma$  discussed below. Collective modes such as long-range spin-fluctuations are not included in the present description.

To study the interplay between local correlations and orbital order we add a small nematic perturbation to the original Hamiltonian Eq. (1) and analyze the linear response of the system. Perturbations in both the  $A_{1g} \sim (n_{xz}(\mathbf{k}) + n_{yz}(\mathbf{k}))$  and  $B_{1g} \sim (n_{xz}(\mathbf{k}) - n_{yz}(\mathbf{k}))$  channels are studied

$$\delta H_{A_{1g}/B_{1g}}^m = \sum_{\mathbf{k}} (n_{xz}(\mathbf{k}) \pm n_{yz}(\mathbf{k})) f_m(\mathbf{k}) h_m \quad (2)$$

$m$  defines the orbital order under consideration,  $f_m(\mathbf{k})$  describes the modulation of the perturbation in momentum space and  $h_m$  is the perturbing field.  $\Delta_m = -\langle \sum_{\mathbf{k}} (n_{xz}(\mathbf{k}) \pm n_{yz}(\mathbf{k})) f_m(\mathbf{k}) \rangle$  is the order parameter associated to each perturbation and  $\chi_m = \delta \Delta_m / \delta h_m$  is

the relative susceptibility. A diverging susceptibility signals a second order phase transition while the suppression of the susceptibility indicates competition between local correlations and nematicity.

Specifically we study:

(a) The  $B_{1g}$  OFO perturbation which lifts the degeneracy of the  $xz/yz$  onsite energy

$$h_{OFO} = \delta\epsilon \quad f_{OFO}(\mathbf{k}) = 1$$

$\Delta_{OFO} = \langle \sum_{\mathbf{k}} (n_{yz}(\mathbf{k}) - n_{xz}(\mathbf{k})) f_{OFO}(\mathbf{k}) \rangle$  is the occupation imbalance between  $xz$  and  $yz$  orbitals [34–36];

(b) The  $B_{1g}$  SCO perturbation given by

$$h_{SCO} = \delta t' \quad f_{SCO}(\mathbf{k}) = \cos k_x \cos k_y$$

that breaks the degeneracy of the intraorbital  $zx$  and  $yz$  second neighbor hoppings. The order parameter  $\Delta_{SCO} = \langle \sum_{\mathbf{k}} (n_{yz}(\mathbf{k}) - n_{xz}(\mathbf{k})) f_{SCO}(\mathbf{k}) \rangle$ , that changes sign between the e- and h-pockets, is compatible with predictions from RG calculations [45];

(c) The  $A_{1g}$  DBO perturbation

$$h_{DBO} = \delta t \quad f_{DBO}(\mathbf{k}) = (\cos k_x - \cos k_y)/2$$

breaks the orbital degeneracy of the intraorbital  $zx$  and  $yz$  nearest neighbor hoppings. Its order parameter  $\Delta_{DBO} = -\langle \sum_{\mathbf{k}} (n_{xz}(\mathbf{k}) + n_{yz}(\mathbf{k})) f_{DBO}(\mathbf{k}) \rangle$  was proposed in connection to ARPES experiments [46, 47, 49, 50].

Below we refer specifically to the case of FeSe. Nevertheless our discussion as a function of  $U$  and main conclusions are valid for other IBS.

### INTERPLAY BETWEEN HUND'S COUPLING AND ORBITAL ORDERS

Fig. 1(a) shows the nematic susceptibilities  $\chi_m$  as a function of  $U$ , normalized to their non-interacting value  $\chi_m^0$ . The OFO susceptibility is strongly suppressed by interactions. This effect closely tracks the strengthening of local correlations, measured by the orbital-dependent quasiparticle weights  $Z_\gamma$  which fall at the same interaction values, see Fig. 1(b). Correspondingly the electronic mass, not shown explicitly, are strongly enhanced at these interactions. The sharp drop of  $Z_\gamma$  evidences the crossover between two metallic states: a low-spin weakly correlated state and a high-spin strongly correlated metallic state [17, 21, 22], the Hund metal. The suppression of the OFO order is prominent at the entrance of the Hund's metal region, as also seen in Fig. 2(a): With increasing  $J_H/U$  the suppression of the order becomes sharper and happens at smaller values of  $U$ , following the evolution of the Hund's metal crossover with  $J_H/U$  [16, 17, 21, 22]. In contrast with  $\chi_{OFO}$ ,  $\chi_{SCO}$  depends weakly on  $U$ , while  $\chi_{DBO}$  is suppressed, but not so strongly as  $\chi_{OFO}$  (Fig. 1(a)).

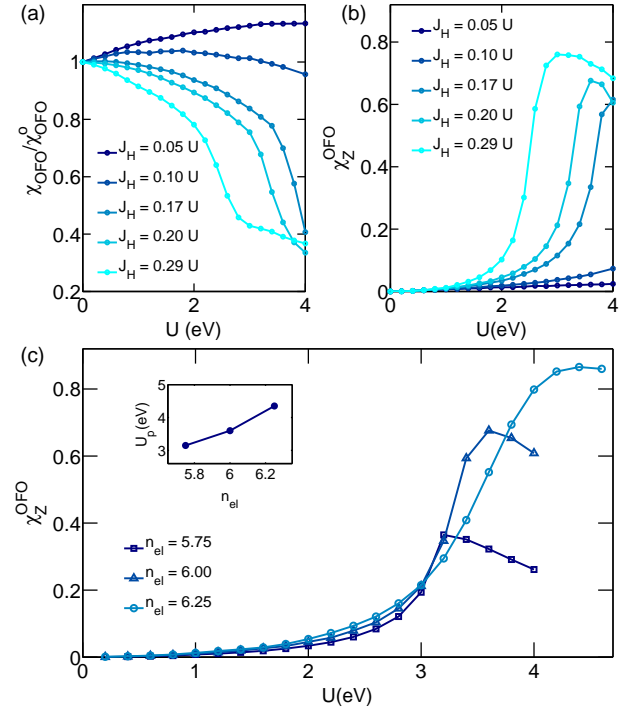


FIG. 2: (Color online) (a)  $\chi_{OFO}(U)$  susceptibility, normalized to its  $U = 0$  value, for  $n = 6$  and different values of  $J_H/U$ . The suppression of the order is prominent and appears at smaller  $U$  for larger  $J_H/U$ . At small  $J_H/U$  the order is not suppressed. (b)  $\chi_Z^{OFO}(U)$  for  $n = 6$  and different values of  $J_H/U$ . (c)  $\chi_Z^{OFO}(U)$  for  $J_H/U = 0.20$  and several  $n$ . In the inset: Interaction  $U_p$  at which  $\chi_Z^{OFO}$  peaks as a function of  $n$ . The peak in  $\chi_Z^{OFO}$  moves towards smaller  $U$  with increasing  $J_H/U$  and decreasing  $n$  following the same dependence than the crossover between the weakly correlated and the Hund metal. The evolution of  $\chi_Z^{OFO}$  shown in panels (b)-(c) is representative also for the DBO and SCO case.

None of the susceptibilities diverge as a function of the interactions. This indicates that the local correlations do not produce by itself the nematic transition. Nevertheless, the different response of the system to each of the orders at the Hund metal crossover found above implies that Hund's physics strongly constraints the nature of the nematic state.

Quantum oscillation and ARPES experiments on FeSe give mass renormalization factors  $m_{zx,yz} \sim 3$  and  $m_{xy} \sim 6 - 9$  [28–30]. From the values in Fig. 1 (b), we estimate  $U \sim 3.5$  eV for FeSe. These mass enhancements place FeSe very close to the Hund metal crossover. For this value of the interaction OFO order is strongly suppressed what practically rules out the possible presence this order. Conversely, local correlations barely affect the SCO making this order a good candidate to explain the nematic state of FeSe.

The different response of the system to the different orders can be traced back to the different occupation imbalance between  $zx$  and  $yz$  orbitals, which is large in the OFO case, intermediate for the DBO and very

small for the SCO perturbation, see Fig. 1(c). Hund's coupling spreads the electrons among the orbitals and therefore strongly suppresses the orders implying a large imbalance. Unequal orbital occupation is suppressed by Hund's coupling because it reduces the spin polarization and increases the intraorbital double occupancy which is energetically unfavorable (see Eq. (1)). Calculations with a different SCO perturbation [57] but with similarly small occupation imbalance give consistent results regarding the weak effect of interactions and support this interpretation.

The differences in the magnitude of the charge imbalance depend on the band reorganization produced by the orbital order close to the Fermi level. The contributions of the e- and h-pockets to the occupation imbalance add in the OFO case, at  $U = 0$  while they partially cancel out in the SCO perturbation.

In the following, we consider that a nematic order is present, assuming that it has been stabilized by degrees of freedom not included here, and analyze the effect of local correlations on the anisotropic properties. For the sake of generality we do not restrict the type of orbital order and consider the three kinds discussed above.

### ANISOTROPIC ORBITAL DIFFERENTIATION AT THE HUND'S CROSSOVER.

In the tetragonal state the  $zx$  and  $yz$  orbitals are degenerate and their quasiparticle weights are equal. A nematic perturbation lifts this degeneracy and leads to different  $Z$ 's, inducing a further source of anisotropy in the observables. A different degree of correlations in  $zx$  and  $yz$  orbitals was early suggested in Hartree-Fock calculations in the  $(\pi, 0)$  magnetic state[18]. However, this effect has been overlooked in the theoretical studies of the nematic state and in the interpretation of the experiments. To analyze this anisotropy we consider a generalized linear response function

$$\chi_Z^m(U) = \frac{\delta(Z_{zx} - Z_{yz})}{\delta h_m}. \quad (3)$$

For each of the three orders,  $\chi_Z^m(U)$  shows a clear peak at the Hund's metal crossover, see Fig. 1 (d). In this region the quasiparticle weight is more sensitive to small perturbations. The spin polarization favors the decoupling of the orbitals as the effective interaction between the electrons in different orbitals is reduced when their spins are parallel [20, 21].

The peak position has the same dependence on the ratio  $J_H/U$  and on the filling  $n$  as the one previously reported for the Hund's metal crossover[9, 16, 17, 21, 22, 59]. The dependence of the peak position can be seen in Fig. 2 (b) and (c) for the OFO case but is common to the three orders. In particular the doping dependence reflects the strong anisotropy between hole and electron

doping, which has been connected with the relevance of the  $n = 5$  Mott insulator on the whole doping phase diagram of the IBS [9, 12, 18, 20, 21, 60].

### BAND SPLITTINGS AT SYMMETRY POINTS

In the unperturbed tetragonal state the  $zx$  and  $yz$  bands at the  $\Gamma$  and  $M$  points are degenerate. The breaking of the  $C_4$  symmetry in the nematic state induces finite splittings  $Sp_\Gamma^m$  and  $Sp_M^m$  between  $zx$  and  $yz$  bands at these points which depend on the nematic order and have been extensively studied in FeSe by ARPES experiments[29, 30, 48–53]. The measured ratio  $Sp_\Gamma^m/Sp_M^m$  and its relative sign have led to conclusions on the kind of orbital order present in FeSe. The interpretation of the experiments has been done assuming the predicted values of the splittings in the absence of interactions:

$$\begin{aligned} Sp_\Gamma^{OFO}(U=0) &= 2\delta\epsilon & Sp_M^{OFO}(U=0) &= 2\delta\epsilon \\ Sp_\Gamma^{SCO}(U=0) &= 2\delta t' & Sp_M^{SCO}(U=0) &= -2\delta t' \\ Sp_\Gamma^{DBO}(U=0) &= 0 & Sp_M^{DBO}(U=0) &= 2\delta t \end{aligned} \quad (4)$$

The renormalization of orbital masses and onsite energies induced by the local correlations modifies the electronic band structure in the nematic phase. In particular, at finite  $U$  an onsite orbital-dependent shift  $\delta\lambda_\gamma$  with  $\lambda_{zx} \neq \lambda_{yz}$  is induced and, as discussed above, the quasiparticle weight is renormalized with  $Z_{zx} \neq Z_{yz}$ , i.e. the mass is different for  $zx$  and  $yz$  orbitals. Both effects renormalize in a momentum-dependent way the band structure defining new  $Sp_\Gamma^m$  and  $Sp_M^m$ , which ratio is qualitatively different with respect the bare ones of Eq. (4). Even if a quantitative comparison with experiments[29, 30, 48–53], at present controversial, is beyond the aim of this work, in the following we discuss qualitatively the change in the splittings  $Sp_\Gamma^m$  and  $Sp_M^m$  induced by local correlations. Not to include the effect of this modification can lead to a wrong interpretation of the experiments.

The primary effect of the correlations is a suppression of the splittings which follows the band narrowing. This reduction of the splitting does not modify the ratio  $Sp_\Gamma^m/Sp_M^m$  nor it implies an equal suppression of the nematic order parameters which are described by  $\chi_m$  in Fig.1(a). In particular, in the SCO and DBO orders the effective nematic hoppings  $\delta t'$  and  $\delta t$  are approximately renormalized by a factor  $\delta Z_{av} \sim (Z_{zx} + Z_{yz})/2$ , being the splittings at  $\Gamma$  and  $M$  corresponding to these orders suppressed by the same factor.

However, there is an extra contribution which affects differently  $\delta Sp_\Gamma^m$  and  $\delta Sp_M^m$  and changes their ratio. This contribution can be approximated by[61]:

$$\begin{aligned} \delta Sp_\Gamma^m &= -\delta\lambda^m + \delta Z^m(2t_{zx,zx}^y + 4t_{zx,zx}'^y) \\ \delta Sp_M^m &= -\delta\lambda^m - \delta Z^m(2t_{zx,zx}^y + 4t_{zx,zx}'^y) \end{aligned} \quad (5)$$

$\delta\lambda^m = \lambda_{zx}^m - \lambda_{yz}^m$  modifies the onsite splitting and  $\delta Z^m = Z_{zx} - Z_{yz}$  induces a momentum-dependent change.

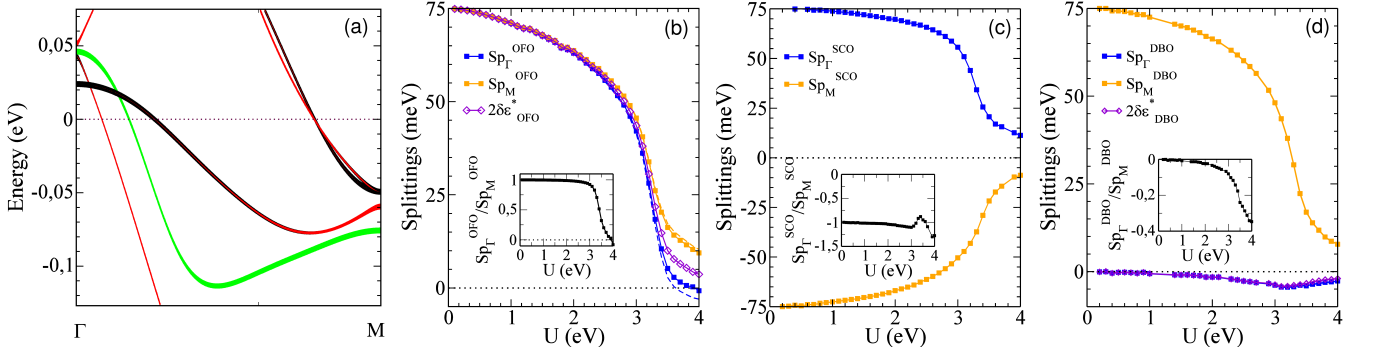


FIG. 3: (Color online) (a) FeSe band structure in the 2Fe Brillouin zone close to the Fermi level along  $\Gamma - M$  for an OFO perturbation  $2\delta\epsilon = 75$  meV and  $U = 3.5$  eV ( $zx$  is indicated in red,  $yz$  in green and  $xy$ ,  $x^2 - y^2$  and  $3z^2 - r^2$  in black). (b)-(d) Splittings at  $\Gamma$  and  $M$ ,  $Sp_\Gamma^m$  (blue) and  $Sp_M^m$  (orange) as a function of  $U$  for the (b) OFO, (c) SCO and (d) DBO perturbations corresponding to  $2h_m = 75$  meV. The renormalized onsite energy splitting for the OFO case (b)  $2\delta\epsilon_{OFO}^* = 2\delta\epsilon - \delta\lambda^{OFO}$  and the DBO one (d)  $2\delta\epsilon_{DBO}^* = -\delta\lambda^{DBO}$  are shown in purple[58]. In (c)  $2\delta\epsilon_{SCO}^*$  is smaller than 3 meV and not shown. Solid lines are guides to the eye. Dashed lines in (b) give the value of the splittings calculated with the approximation in Eq. (5). With interactions the relative ratio of the splittings, shown in the insets, changes. The different value of  $Sp_\Gamma^{OFO}$  and  $Sp_M^{OFO}$  in (b) is due to the different value of  $Z_{zx}$  and  $Z_{yz}$ . On the other hand the finite value of  $Sp_\Gamma^{DBO}$  in (d) is primarily accounted for by the change in the onsite energies  $2\delta\epsilon_{DBO}^*$ . Spin-orbit interaction, not included here, will further modify the splittings at  $\Gamma$  [27].

In order to highlight the different evolution of the splittings at  $\Gamma$  and  $M$  under the different perturbations we use a numerical value  $2h_m = 75$  meV. Fig. 3(a) shows the band dispersion along  $\Gamma - M$  for the OFO perturbation and  $U \sim 3.5$  eV. The splitting at  $M$  is much larger than the one at  $\Gamma$  which almost vanishes. This is contrary to the equal value of the bare splittings  $Sp_\Gamma^{OFO} = Sp_M^{OFO}$  of Eq. (4) assumed in previous works to interpret ARPES experiments.

The evolution with interactions of  $Sp_\Gamma^m$  and  $Sp_M^m$  and their ratio for the three orders is plotted in Figs. 3(b-d). A primary effect of the correlations is to decrease the size of the splittings, as expected from the renormalization of the bands. Less obvious is the  $k$ -dependence of the renormalization introduced by interactions, that makes the correlated ratios  $Sp_\Gamma^m / Sp_M^m$ , shown in the insets of Figs. 3(b-d), different from the bare ones. This effect is mostly due to the differentiation of the  $zx/yz$  spectral weight  $\delta Z^m \neq 0$ , see Eq. 5. The splittings  $Sp_\Gamma^m$  and  $Sp_M^m$  and their ratio  $Sp_\Gamma^m / Sp_M^m$  are especially sensitive to the interactions at the Hund's metal crossover. Nevertheless,  $Sp_\Gamma^m / Sp_M^m$  is affected differently for the different orders. This ratio is weakly affected in the SCO. On the contrary in the OFO and DBO cases, the interactions renormalize differently the band structure at  $\Gamma$  and  $M$  and can even produce accidental sign-change between the splittings at the electron and hole pockets, as for example in Fig. 3(b).

## SUMMARY AND DISCUSSION

In this work, we have shown that local correlations, and in particular, Hund's physics, have a strong impact on orbital orders states. The sensitivity is largest for in-

teraction values at the Hund's metal crossover. The mass renormalization factors observed experimentally [28–30], place this material at the entrance of the Hund's metal where we find a more pronounced sensitivity of the nematic properties to local correlations. At these values of the interactions we find the largest difference between the quasiparticle weight of  $zx$  and  $yz$  material, what makes that these two orbitals present different band mass. For the perturbation used in the splitting analysis,  $2h_m = 75$  meV, that gives  $M$  splittings of the order of 20 meV at values of the interactions relevant for FeSe ( $U \sim 3.5$  eV,  $J_H/U = 0.20$ ), we found a differentiation  $\delta Z^{OFO} \sim 0.025$  where the unperturbed  $Z_{zx/yz} \sim 0.26$ . This corresponds to a variation of the 9.5%, that reduce to the 3.2% and 1.5% for the SCO and DBO cases respectively.

While the effect of local interactions may look small on a first sight, it has strong implications on observable properties, like the splittings  $Sp_\Gamma^m$  and  $Sp_M^m$  between the  $zx$  and  $yz$  bands at  $\Gamma$  and  $M$  measurable by ARPES. It modifies their ratio and may even modify their sign. While in the absence of interactions the splittings at  $\Gamma$  and  $M$  are expected to be equal for the onsite OFO order, for interaction values relevant in FeSe the splitting at  $\Gamma$  is strongly reduced with respect to the value at  $M$ . In the d-wave nematic bond order DBO, the splitting at  $\Gamma$ , zero in the absence of interactions, acquires a finite value approximately 1/3 of the splitting at  $M$  and opposite sign. The relative sign of the splittings is less affected in the case of a sign-changing SCO order. The modification of the splittings induced by local correlations has to be taken into account in order to correctly interpret the ARPES spectra.

From the analysis of the orbital response, we did not

find any evidence of divergence of the orbital nematic susceptibilities  $\chi_m$  and therefore no signature of the associated phase transitions. This means that the nematic transition must be either mediated or at least assisted by degrees of freedom not included here, e.g. spin fluctuations. Nevertheless, our study demonstrates that Hund's physics strongly constraints the nature of a possible orbital ordered state realized in the nematic phase suppressing any order generating large  $zx/yz$  charge imbalance as the onsite ferro-orbital ordering OFO. On the contrary a sign-changing orbital order SCO, with small charge imbalance between  $zx$  and  $yz$  orbitals, is only weakly affected by interactions. Thus SCO emerges as the most likely candidate to be realized in the nematic phase of FeSe. This order was proposed to be stabilized, by spin fluctuations on the basis of parquet renormalization group calculations[45]. In fact, the modification of the splittings at  $\Gamma$  and  $M$  produced by the correlations happens to reduce the difference in occupation between  $zx$  and  $yz$  orbitals. A similar tendency is derived via orbital-selective self-energy[52] and vertex corrections[62].

While we have focused on FeSe, our description is not restricted to this compound. The smaller mass enhancement measured for iron pnictides with respect to FeSe suggest that the effect of the Hund's physics on the nematic state of FeAs compound should be present, even if less pronounced than in FeSe.

Note added: After we submitted this article for the first time the preprint[63] was posted on the arXiv. In this work the Quasiparticle Interference spectrum is fitted using a multi-orbital RPA approach which uses the quasiparticle weights as fitting parameters. Interestingly different values for  $Z_{zx}$  and  $Z_{yz}$  are allowed. However, a very large difference between  $Z_{zx}$  0.16 and  $Z_{yz}$  0.8 is obtained from these fittings. Such a large difference cannot be accounted for by local correlations. In fact if such difference between the mass of these orbitals were associated to a renormalization of the hopping parameters the electronic bandstructure would dramatically be modified and this is not observed experimentally.

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